Mathematical Models and Methods for Ab Initio Quantum Chemistry

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Book Condition: New. Publisher/Verlag: Springer, Berlin | On the occasion of the fourth International Conference on Industrial and Applied Mathematics!, we decided to organize a sequence of 4 minisymposia devoted to the mathematical aspects and the numerical aspects of Quantum Chemistry. Our goal was to bring together scientists from different communities, namely mathematicians, experts at numerical analysis and computer science, chemists, just to see whether this heterogeneous set of lecturers can produce a rather homogeneous presentation of the domain to an uninitiated audience. To the best of our knowledgde, nothing of this kind had never been tempted so far. It seemed to us that it was the good time for doing it, both . because the interest of applied mathematicians into the world of computational chemistry has exponentially increased in the past few years, and because the community of chemists feels more and more concerned with the numerical issues. Indeed, in the early years of Quantum Chemistry, the pioneers (Coulson, Mac Weeny, just to quote two of them) used to solve fundamental equations modelling toy systems which could be simply numerically handled in view of their very limited size. The true difficulty arose with the need to model larger systems...

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